Automated Data Interpretation Standard Laboratory Module (SLM™)

General Overview of the Automated Data Interpretation SLM

Initially, the Data Interpretation Module (DIM) is being developed to automate the interpretation of gas chromatograms (GCs) for organochlorine compounds and polychlorinated biphenyls (PCBs). Complex mixtures of PCBs were manufactured and sold in the U.S. under the Aroclor trade name. The analyses of chromatograms for Aroclors, petroleum hydrocarbons, and other multicomponent materials are among the most difficult analyses to perform. Current manual data interpretation practice for an unknown Aroclor sample requires a human comparison of the unknown chromatogram with that obtained from a standard sample.

Environmental Protection Agency (EPA) Method

EPA Method 8080

Standard Analysis Method (SAM)

This model, when complete, will accomplish the data analysis of organic compounds listed in Method 8080.

Advantages

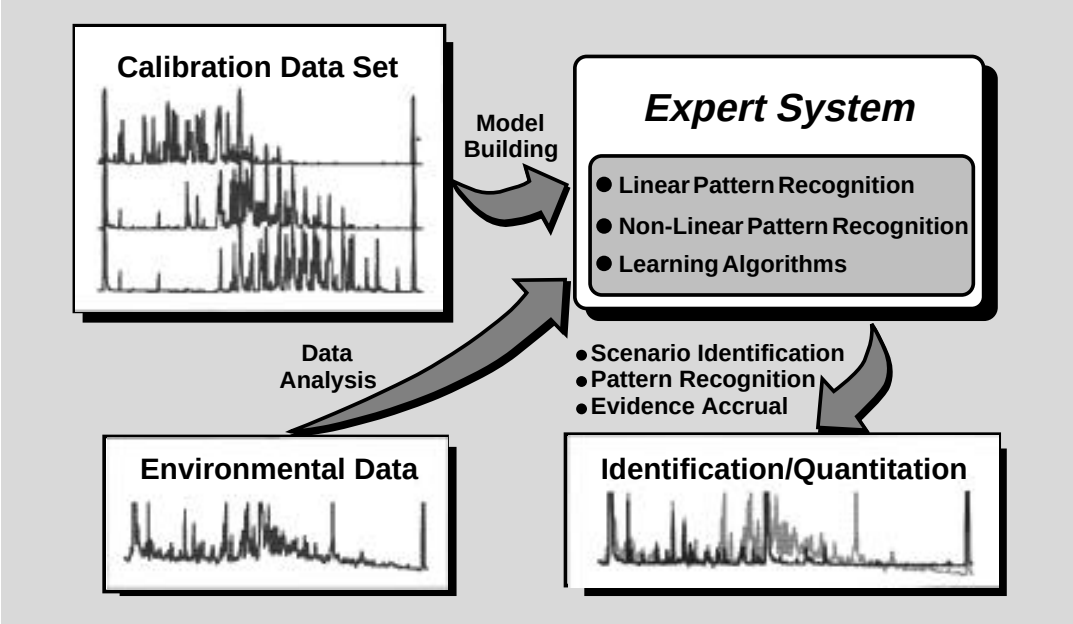
In addition to decreased time, increases in accuracy and reproducibility are realized through integration of the module's data processing techniques.

Case	Manual Analysis Time	Automated Analysis Time
No Aroclor Contamination	0-1 minute	5-10 seconds
Single Aroclor Contamination	0-2 minutes	5-10 seconds
Multiple Aroclor Contamination	15-30 minutes	5-10 seconds

General Description of the Automated Data Interpretation SLM

Pattern recognition data processing techniques are required in order to replace the intuitive pattern recognition performed by chemists on multicomponent target analytes. This project has developed and applied principal component regression, multiple linear regression analysis, and neural network pattern recognition to this problem. An expert system strategy uses the data processing results and knowledge

Figure 1. Automated chromatography data interpretation.



Robotics Technology Development Program

about the capabilities of the data processing methods to create a final result.

The current methods automated under the expert system are developed to identify Aroclors from their chromatographic profile in GCs. Using pattern recognition tools, chemists can easily develop tools to identify other compounds from the raw chromatographic data.

Status

A software system has been developed that will carry out automated GC data interpretation for commercial Aroclors and Aroclor mixtures. Standard chromatography data analysis methods as well as novel pattern recognition methods have been incorporated into the system.

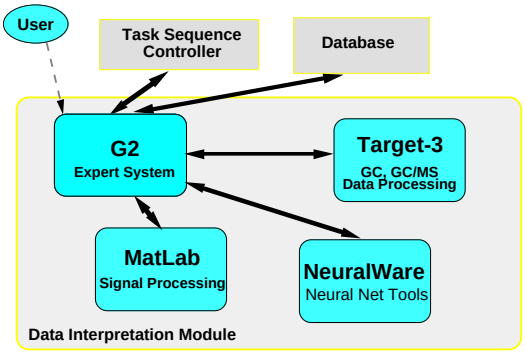


Figure 2. Functional diagram of the DIM.

Industrial Partners

Thru-Put Systems Inc., of Orlando, Florida, produces UNIX-based GC and GC/MS data processing software. They are working through a Cooperative Research and Development Agreement (CRADA) with the Contaminant Analysis Automation Program to develop and commercialize the pattern recognition tools developed for multicomponent analysis.

Neural Ware Inc. of Pittsburgh, Pennsylvania, is working through a CRADA with Los Alamos National Laboratory to develop neural network pattern recognition tools for chromatography data processing.

Developers

Los Alamos National Laboratory, Oak Ridge National Laboratory, and University of Tennessee/Knoxville.

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